Fundamentals of Combustion for Propulsion

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Lecture - 10
Conservation equations

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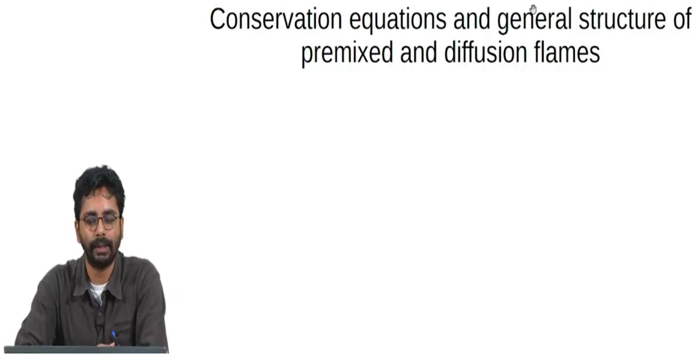

Conservation equations and general structure of premixed and diffusion flames

Welcome back. Yesterday in the previous lectures, we discussed several commonalities and differences between combustion systems. And in that discussion some fundamental aspects of flame structure and its dependence on reaction rate or transport processes or combination of these were also discussed. What we will do today is introduce the formal structure which enables computation of precise flame structures ok. These formal equations are nothing but the conservation equations ok. So, we will quickly go over the basic conservation equations and then the equations in one dimensional form and then look at the connections between the general ideas that were introduced yesterday and the conservation equations.

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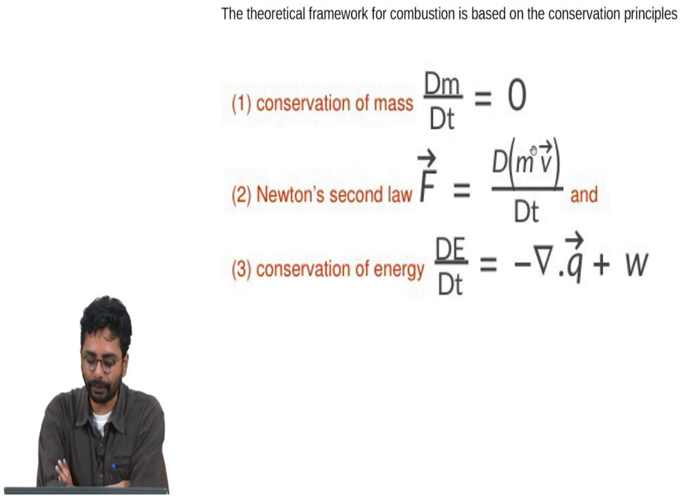

The theoretical framework for combustion is based on the conservation principles

(1) conservation of mass $\frac{Dm}{Dt} = 0$

(2) Newton's second law $\vec{F} = \frac{D(m\vec{v})}{Dt}$ and

(3) conservation of energy $\frac{DE}{Dt} = -\nabla.\vec{q} + W$

So, the theoretical framework for combustion is based on the conservation principles. There are one there are 3 conservation principles: one is conservation of mass and then Newton's second law which relates force and changes in momentum and conservation of energy. So, the conservation of mass is in combustion systems mass is either created nor destroyed. So, if we choose a packet of certain mass and track it in time, then the change in mass will be 0 that is what is expressed as Dm by Dt is 0 ok. Newton second law, you all know that if the same parcel of mass that we are tracking the motion of that is controlled by the Newton's second law is governed by the Newton second law.

So, it states that the force is the rate of change of momentum and both force and momentum are vector quantity. So, this is in Cartesian coordinates, this will be essentially three equations for each component of velocity. And conservation of energy is statement of the first law of thermodynamics which we used yesterday which states that if you track a parcel of mass, the total energy of that mass will change because of two things. One is when heat is transferred to or out of that mass and the other is because of work done on that mass ok. So, all phenomena that we have been discussing are governed by these principles.

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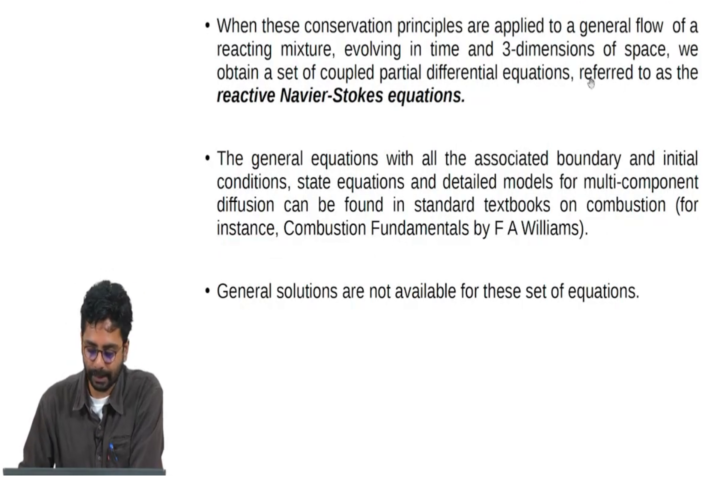

- When these conservation principles are applied to a general flow of a reacting mixture, evolving in time and 3-dimensions of space, we obtain a set of coupled partial differential equations, referred to as the ***reactive Navier-Stokes equations.***
- The general equations with all the associated boundary and initial conditions, state equations and detailed models for multi-component diffusion can be found in standard textbooks on combustion (for instance, Combustion Fundamentals by F A Williams).
- General solutions are not available for these set of equations.

So, when these conservation principles are applied to a general flow of reacting mixture which can change in time and also in 3-dimensions of space. We obtain a set of couple partial differential equations referred to as a reactive Navier-Stokes equations.

The general equations, the reactive Navier-Stokes equation with all the associated boundary and initial conditions, state equations to relate pressure with temperature and density and concentration of reactants and products and detailed models for multi component diffusion. Because in a reacting flow situation you may have areas or parts of the flow where the concentration of reactants are higher than the concentration of the products and vice versa in some other zones ok, in neighboring zones and therefore, this concentration gradients will drive mass diffusion ok.

So, we need models for accounting for the mass transfer because of concentration gradients which is usually done or assume to follow Fick's law of diffusion. And in the simple form it is assumed to follow Ficks law of diffusion. Sometimes when you have to you may have to account for a more detailed diffusion model to explain some phenomena ok.

So, detailed models for multi component diffusion, I will find these equations along with diffusion models and reaction models of variety of complexity and hierarchy and standard textbooks, for example, Combustion Fundamentals by F A Williams ok. Important thing is that general solutions are not available for the set of equations and therefore, that is the reason why we need simpler models and identification of controlling parameters, so that we will can construct the simplified description of the process.

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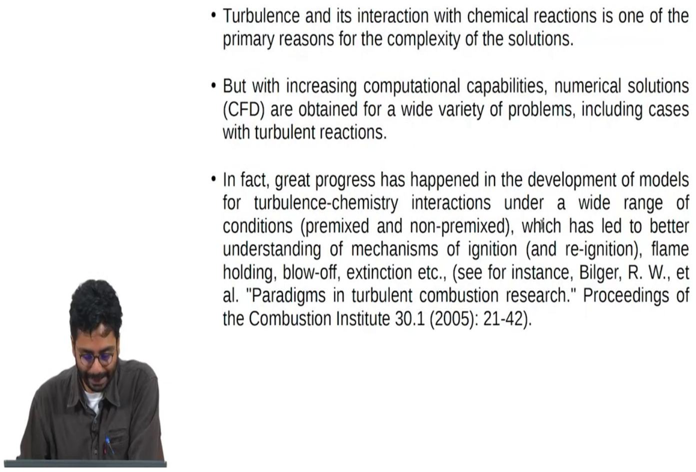

- Turbulence and its interaction with chemical reactions is one of the primary reasons for the complexity of the solutions.
- But with increasing computational capabilities, numerical solutions (CFD) are obtained for a wide variety of problems, including cases with turbulent reactions.
- In fact, great progress has happened in the development of models for turbulence-chemistry interactions under a wide range of conditions (premixed and non-premixed), which has led to better understanding of mechanisms of ignition (and re-ignition), flame holding, blow-off, extinction etc., (see for instance, Bilger, R. W., et al. "Paradigms in turbulent combustion research." Proceedings of the Combustion Institute 30.1 (2005): 21-42).

One of the reasons why it is we do not have general solutions for these set of equations is because of the turbulence and its interaction with the reactions and flame.

So, turbulence and its interaction with chemical reactions is one of the primary reasons for the complexity of the solutions. Of course, these days we have computational capabilities and therefore, we can get numerical solutions for a wide variety of problems including cases with turbulent reactions. In fact, lot of progress has happened in the development of models for turbulence chemistry interactions including for pre mixed and non premixed and partially pre mixed conditions which is led to better understanding of mechanisms of ignition and re ignition something that was discussed yesterday. That flames can locally become extinct in a complex turbulent flow and it can reignite a while later ok.

All these phenomena can now be accurately captured using computational tools ok, flame holding blow of extinction etcetera are all possible to compute using by numerically solving the conservation equations.

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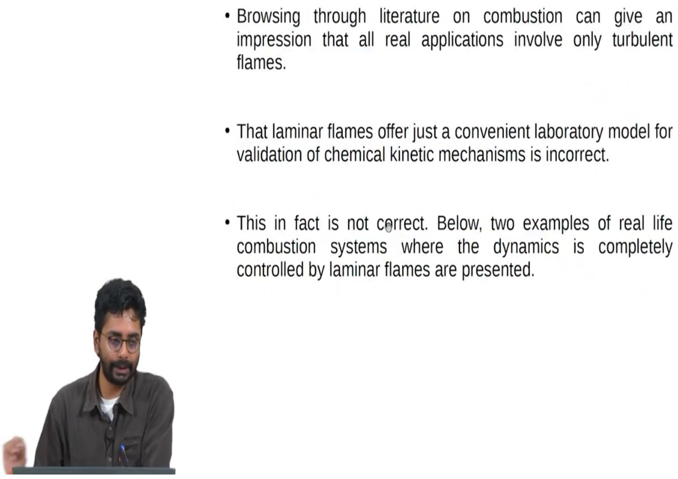

- Browsing through literature on combustion can give an impression that all real applications involve only turbulent flames.
- That laminar flames offer just a convenient laboratory model for validation of chemical kinetic mechanisms is incorrect.
- This in fact is not correct. Below, two examples of real life combustion systems where the dynamics is completely controlled by laminar flames are presented.

But there is something important that I wanted to bring up and discuss. If you look at the top journals in the field of combustion for example, combustion and flame or proceeding, so, the combustion institute. So, browsing through these journals on combustion can give you an impression that that turbulent combustion is the norm and laminar flames are exceptions ok.

A similar statement is also made in you know courses in fluid mechanics that laminar flames laminar flow is exception and turbulence is the norm. And that laminar flames are helpful only because they offer a convenient laboratory model for validation of chemical kinetic mechanisms is the impression that one might get browsing through literature, but this is not correct. I will show you two examples of real life combustion systems where the dynamics is completely controlled by laminar flames.

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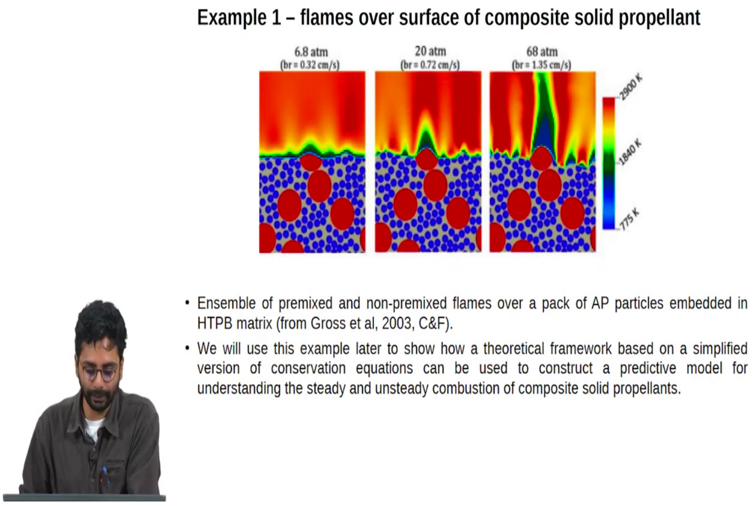

Example 1 – flames over surface of composite solid propellant

- Ensemble of premixed and non-premixed flames over a pack of AP particles embedded in HTPB matrix (from Gross et al, 2003, C&F).
- We will use this example later to show how a theoretical framework based on a simplified version of conservation equations can be used to construct a predictive model for understanding the steady and unsteady combustion of composite solid propellants.

The first example is flames over surfaces of composite solid propellants. I think they should explain this figure in some detail. What you see here is a cross section of a propellant cross section of an AP HTPB propellant which contains two sizes of AP particles, one large the red color one and one small. The red color one, the red colored particles are 200 micron in diameter and the blue color ones are 12 micron in diameter and they are embedded in a matrix of fuel ok.

That is how that is a general structure of a solid propellant; you have oxidizer and fuel mixed together and the oxidizer embedded in a matrix of fuel ok. What is shown here is a CFD simulation of the flame structure over such a composite propellant.

The solution the CFD solution is shown for three different pressures; one at 6.8 atmospheres, now there are 20 atmospheres and at 68 atmospheres ok. The of course, you can see that there are a lot of differences between there is a lot of change in the frame structure as a pressure changes with the same structure of the propellant. The structure of the propellant that you see at the bottom are the same, but the structure of the flame on top changes with pressure ok.

The general structure of the flame over composite solid propellants can be described as an ensemble of pre mixed and non pre mixed flames ok, over a pack of AP particles embedded in HTPB matrix ok. The pre mixed flames are formed over the surface of AP which is ammonium perchlorate which is a mono propellant, like hydrazine it can burn on its own. It can undergo a self sustained deflagration. So, AP has a pre mixed mono propellant flames sitting right on top of it and AP is surrounded by fuel ok. AP is an oxidizer rich mono propellant. So, it will exothermically decompose give off a large amount of oxygen; actually the decomposition products of ammonium perchlorate will have about 32 percent oxygen.

So, what ammonium perchlorate; the way ammonium perchlorate burnt since it will have a flame over top of it which will burn the decomposition products of ammonium perchlorate and what comes out is a stream containing 32 percent oxygen. And this stream of oxidizer which gases is surrounded by a stream of decomposition products of fuel or essentially fuel vapors ok. So, the fuel vapors; so, now, you have oxygen coming from the center fuel coming from the side and this can form a non pre mixed flame.

So, what you see here is premix flames over AP surfaces surrounded by non premix flames formed by reaction between AP and HTPB ok. So, what is happening as the pressure increases is remember that pre mixed flames under these conditions are essentially flat one dimensional flames over the surface of AP ok. So, what is happening as a pressure increases is that the structure of the flame is changing. It looks as if the height of the diffusion flame is increasing and its influence over the burn rate is decreasing. This is the qualitative behavior which more precisely will be discussed later ok.

So, as I mentioned we will use this example later to show how a theoretical framework based on simplified version of conservation equations can be used to construct a predictive model for understanding the steady and steady conversion of composite solid propellants. This is one example and of course, it goes without saying that this is an example where the flame over the surface is completely laminar, as I said the size of this red color circle is about 200 microns and the flame standoff distance is at the maximum a few 10s of microns.

So, if you use this length scale and velocity scale, the velocity of the gases that come out from the surface is a few meters per second and we use this length scale and the velocity scale along with viscosity under these conditions. You can calculate the Reynolds number and show that the flow in these three cases are well within the laminar regime ok.

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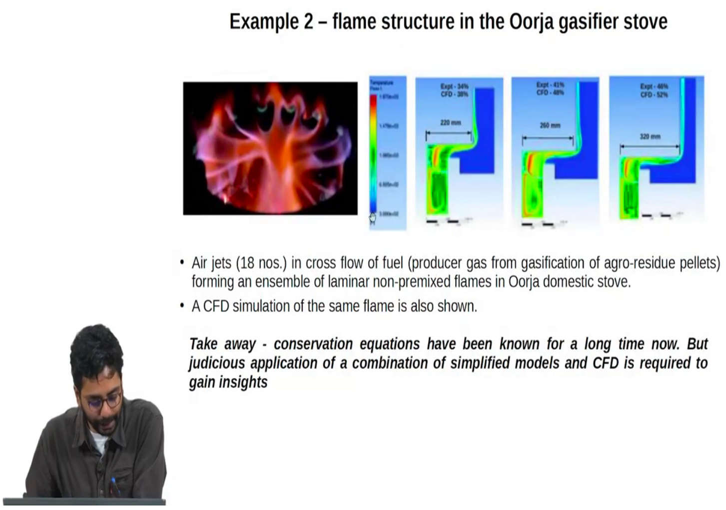

Example 2 – flame structure in the Oorja gasifier stove

- Air jets (18 nos.) in cross flow of fuel (producer gas from gasification of agro-residue pellets) forming an ensemble of laminar non-premixed flames in Oorja domestic stove.
- A CFD simulation of the same flame is also shown.

Take away - conservation equations have been known for a long time now. But judicious application of a combination of simplified models and CFD is required to gain insights

The other example I wanted to show is flame structure in what is called Oorja gasifier stove. What you see here in the picture on the left is what is called a jet in cross flow flame. There is a jet there is a stream of fuel gases that are coming in this direction in the vertical direction and there are this stream is surrounded by 18 holes which are issuing air and flame that you see is formed between the fuel gases that are moving in the vertical direction with the air that is coming from the cross flow direction ok.

So, air jets 18 air jets in cross flow of fuel. So, you have fuel coming like this and oxidizer jets coming like this and this is the flame structure that is formed ah. So, 18 air jets in cross flow of fuel which is nothing, but producer gas from gasification of biomass it forms an ensemble of laminar non prime exclaims in the Oorja stove. And here of course, we heat transfer this is used for domestic cooking and the heat transfer from the flame to the vessel and pollutant formation and heat transfer aspects everything is controlled by laminar flames.

Here again you can calculate of course, it is easy to see from the picture of the flame itself that it is laminar. Of course, you can get estimates for Reynolds number and show it is laminar. Another thing that can be done and that was done is you can get you can make temperature measurements of temperature measurements with time for this flame, calculate the spectra and it can be shown that the spectra corresponds to a unsteady laminar flow and it is not a turbulent flow. And a CFD simulation of the same flame with the effect of the vessel included is shown on the right and comparison between the experimentally measured efficiency and the CFD the efficiency computed from CFD is also shown it matches very well.

So, the these examples I wanted to show just to emphasize that conservation equations have been known for a long time, but judicious application for combinational simplified models and CFD is required to gain insights. And it is important to recognize that there are situations where laminar flames are a good laminar flames control the dynamics and much can be learned by using these principles to judiciously, yes.

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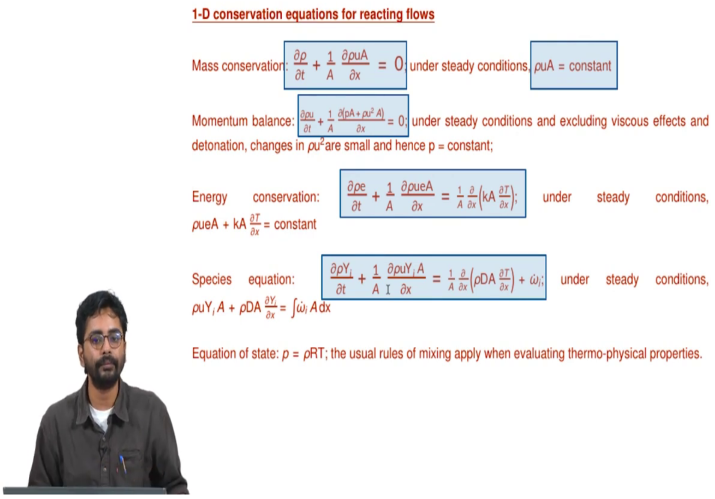

1-D conservation equations for reacting flows

Mass conservation: $\boxed{\frac{\partial \rho}{\partial t} + \frac{1}{A}\frac{\partial \rho u A}{\partial x} = 0}$; under steady conditions, $\boxed{\rho u A = \text{constant}}$

Momentum balance: $\boxed{\frac{\partial \rho u}{\partial t} + \frac{1}{A}\frac{\partial (pA + \rho u^2 A)}{\partial x} = 0}$; under steady conditions and excluding viscous effects and detonation, changes in ρu^2 are small and hence p = constant;

Energy conservation: $\boxed{\frac{\partial \rho e}{\partial t} + \frac{1}{A}\frac{\partial \rho u e A}{\partial x} = \frac{1}{A}\frac{\partial}{\partial x}\left(kA\frac{\partial T}{\partial x}\right)}$; under steady conditions, $\rho u e A + kA\frac{\partial T}{\partial x} = \text{constant}$

Species equation: $\boxed{\frac{\partial \rho Y_i}{\partial t} + \frac{1}{A}\frac{\partial \rho u Y_i A}{\partial x} = \frac{1}{A}\frac{\partial}{\partial x}\left(\rho DA\frac{\partial T}{\partial x}\right) + \dot{\omega}_i}$; under steady conditions, $\rho u Y_i A + \rho DA\frac{\partial Y_i}{\partial x} = \int \dot{\omega}_i A\,dx$

Equation of state: $p = \rho RT$; the usual rules of mixing apply when evaluating thermo-physical properties.

Student: What are the definition of efficiency in the (Refer Time: 14:18)?

The definition of efficiency here is the mass flow rate is the heat transferred to the vessel per unit time divided by the mass flow rate of the fuel multiplied by the calorific value of the fuel, this thermal efficiency. So, with that I will quickly go through conservation equations in simplified forms. You may have gone through derivation of these equations in your fluid mechanics class.

So, the mass conservation principle remember that Dm by Dt is equal to 0, that if you track a parcel of mass m its mass will not change as it goes through the flow field. When expressed in non-linear format will be in this form ah. The first term is the rate of change of mass inside a small control volume and the second term is the net outflow of mass that goes out of the control volume ok. In a simple control volume analysis, you can with the simple control volume analysis you can derive this equation.

So, what it essentially states is that if you look at a control volume the rate of change of mass inside the control volume should be equal to the difference in the mass that enters minus the difference the difference in the mass that enters and leaves ok. Under steady condition; that means, when the mass inside the control volume is not changing with time, this equation will simply reduce to the more familiar form which is density times velocity area is equal to constant ok.

This is the momentum balance in one dimension. The first term is again the rate of change of momentum inside the control volume and the second term is the combination of net outflow of momentum flux and the forces acting on the control volume. Here for simplicity I have ignored the stresses and forces because of viscous effects. I have included only the 4 pressure terms. ah

What is important here is under steady conditions; that means, the first term in the equation is 0 and excluding viscous effects and detonation. Detonation involves shockwaves, supersonic flows and large changes in pressure. If we exclude these situations, this equation will essentially reduce to a condition where pressure is constant. Remember that we use this condition yesterday when we did equilibrium calculations for a methane air pre mixed flame that the pressure is everywhere roughly the same is follows from this idea.

So, you can see that under steady conditions and if the cross section area is not changing with location then we have p plus rho u squared equals constant ok. Remember that velocity scale for a laminar flame hydrocarbon air laminar flame is 0.4 meters per second and density let us say is about 1 kilogram per meter cube. So, if you take density to be 1 kilogram per meter cube and you the velocity to be about 0.4 meters per seconds rho u squared would be 0.16 Pascal's. So, 0.16 Pascal's compared to an atmospheric pressure of 1013 to 5 is very small and that is the reason why we assume that the pressure everywhere is approximately the same ok.

Again similar forms for energy conservation, the first term is the unsteady term; the rate of change of energy inside a control volume. The second term is the net outflow of energy and this is controlled by heat transfer we have missed the work done by the pressure term, but let us say because of this assumption that term is not important ok. So, under steady conditions, we will have the total energy change is only because of heat transfer into and out of a small control volume ok. These are these are these three are equations that you would have seen in your fluid mechanics and heat transfer classes.

What is new in the context of combustion is the species equation. Remember that the concentration is not uniform because of chemical reactions happening in a domain the concentration of species will change both with time as well as spatial location ok.

So, it is important to keep; it is required to keep track of the concentration of different components or different species as a function of time and space and so, this is a balance equation for species concentration ok. The species concentration can change because of the flow which is described by this term. This is the species concentration change because of convection. This is the species concentration change. I am sorry this must be partial Yi by partial x.

This is the species concentration change because of diffusion and D is the diffusion coefficient, it is a binary diffusion coefficient. And what is unique to combustion is that the concentration of the species can change because of chemical reactions. This is what is included here is this effect is included to the omega dot item ok.

So, at a given location in space and at a given as a function of time, the concentration can change because of the flow bringing in some reactants and flow taking out some reactants or mass diffusion because of gradients in concentration at that place and more importantly it can change because of the reactant getting consumed because of chemical reaction or product forming because of you know chemical reactions ok. So, under steady conditions, this is this will simply become the convective term plus the diffusive term balanced by the reaction term ok.

In addition to all of this we need one more equation to relate the thermodynamic variables, this is done through the equation of state that the gases follow the ideal gas equation is reasonably accurate for a variety of situations in combustion and propulsion, of course, except when you are dealing with propulsion systems where you have reactants entering at critical conditions, where you need to be careful and use appropriate equations of state. But for most combustion systems gas turbines and internal combustion engines, this is a very good approximation in the gas phase and the usual rules of mixing apply when evaluating thermo physical properties.

Remember that you have a mixture of gases, you need to appropriately define values for cp values for gamma and other thermo physical properties and also transport properties like thermal conductivity and diffusion coefficients must be properly defined for a mixture of gases and variety of simplifications are usually done. I will just mention one simplification with respect to choice of diffusion coefficients.

In combustion systems where air is used as an oxidizer, the dominant species will be nitrogen because remember that the stoichiometric ratio is about 16 or 17. So, for every gram of fuel that you introduce into the combustion chamber, there are 17 times more air and about 78 percent of air is nitrogen.

So, if you look at a combustion chamber and do a mass budget of various species; oxygen, nitrogen, carbon dioxide and water vapor. I think an example of it was shown yesterday nitrogen will be the dominant species. So, one approximation that is made when choosing diffusion coefficients is to assume that every other species is diffusing into nitrogen. So, you can pick the binary diffusion coefficient for a fuel into nitrogen or carbon dioxide into a nitrogen and that turns out to be a very good approximation for a variety of problems. Any questions so far before we move on to the integral analysis? Yeah.

Student: In the energy equation, equation it seems that there is no reaction of a chemical.

Yes that is a good question. Remember that the definition of energy e or e written as enthalpy minus pv, the enthalpy will be defined including the formation enthalpy and the sensible enthalpy. And once you can actually ah by substituting that definition of enthalpy or internal energy as formation component plus the sensible component into this equation, you will recover an energy release down because of combustion which would which would have the following form it will look like this.

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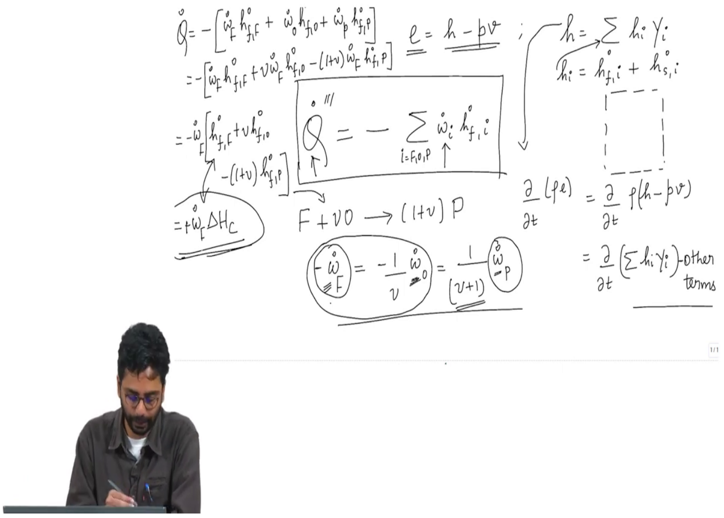

$$\dot{Q} = -\left[\dot{\omega}_F h^0_{f,F} + \dot{\omega}_O h_{f,O} + \dot{\omega}_P h^0_{f,P}\right]$$

$$= -\left[\dot{\omega}_F h^0_{f,F} + \nu\dot{\omega}_F h^0_{f,O} - (1+\nu)\dot{\omega}_F h^0_{f,P}\right]$$

$$= -\dot{\omega}_F\left[h^0_{f,F} + \nu h^0_{f,O} - (1+\nu) h^0_{f,P}\right]$$

$$= +\dot{\omega}_F \Delta H_C$$

$$\boxed{\dot{Q}''' = -\sum_{i=F,O,P} \dot{\omega}_i h^0_{f,i}}$$

$$F + \nu O \longrightarrow (1+\nu) P$$

$$\dot{\omega}_F = -\frac{1}{\nu}\dot{\omega}_O = \frac{1}{(\nu+1)}\dot{\omega}_P$$

$$e = h - pv \; ; \quad h = \sum h_i Y_i$$

$$h_i = h^0_{f,i} + h^0_{s,i}$$

$$\frac{\partial}{\partial t}(\rho e) = \frac{\partial}{\partial t}\rho(h - pv)$$

$$= \frac{\partial}{\partial t}\left(\sum h_i Y_i\right) - \text{other terms}$$

I leave it as an exercise ok, when return in sensible when you split the e.

Student: Is it any formation enthalphy?

Yes, it is only the formation enthalpy.

Student: (Refer Time: 23:45).

The, so, the I have written an equation for e in the conservation equation; we express e as h minus pv. Now, the enthalpy is at enthalpy at let us say assume a control volume, this can have a mixture of species ok. So, the enthalpy of enthalpy content of this control volume will be sum of enthalpy of all the components that are present inside ok, h i into the mass fraction of that component. And each one of these hi’s the enthalpy of a component I, for example, enthalpy of carbon dioxide will be the enthalpy of formation of that component i plus the sensible enthalpy.

So, once you substitute this back here and this definition of h into the energy conservation equation for example, you have a term like this, rho e will become and so on.

Student: (Refer Time: 24:57).

I am sorry yeah, h minus pv. So, now, this h will become some of h i Y i plus or minus other terms and some more algebraic manipulation is required. You need to multiply the species conservation equation by formation enthalpy sum over it and subtract it from here, you will recover equivalent of a chemical heat release term which let us call as Q dot triple dash will have this following form ok.

We will look at a simple case of where this is we will derive a simple equation for this something yeah or maybe right away ah.

Student: Sir this energy equation (Refer Time: 25:55).

This is the reaction rate term; this is the reaction rate term. I just will give a simple demonstration of what this equation means. Let us consider a simple reaction where fuel plus 1 gram of fuel plus nu grams of oxidizer gives you 1 plus nu grams of products ah. If this is the only reaction that is allowed and let us say there is no reverse reaction, it is a irreversible one step reaction, so, for every gram of fuel that is consumed ok. This much of the oxidizer consumed must be nu times the fuel consumed because that is constrained by the stoichiometry and it should result in the formation of this much of products.

I will just explain what this equation one more time; w dot omega dot o is the rate of consumption of the oxidizer. The rate of consumption of the oxidizer must be equal to nu times the rate of consumption of fuel that is what is expressed by this part of the equation ok. Rate of consumption of oxidizer should be nu times rate of consumption of fuel and when omega dot F amount of fuel is consumed, it should result in the formation of new plus 1 times products ok. So, if this much of fuel is consumed the amount of product that will form will be nu plus 1 times that and this equation simply, expresses that right ok.

Now, omega dot i, here i stands for if this is the reaction that we are looking at; i stands for fuel oxidizer and products correct. So, now, you can express this equation for Q in terms of any one of these variables. I will choose fuel because what we are more familiar with is the calorific value of the fuel ok. So, if you substitute or if you expand this by substituting these terms into that equation, you will have Q dot is equal to negative of omega dot F into enthalpy of formation of the fuel plus omega dot o enthalpy of formation of the oxidizer plus omega dot p times enthalpy of formation of the product ok.

So, this now we can use this relationship between this relationship between omega dot F omega dot o and omega dot p which will make this as omega dot F enthalpy of formation of the fuel minus omega dot o is nu times omega dot f. So, this is nu times omega dot F enthalpy of formation of p oxidizer and omega dot p is negative nu plus 1 omega dot F.

So, this is negative 1 plus nu omega dot F enthalpy of formation of the products ok. Now you can combine the terms. This is negative omega dot F h f 0 of the fuel plus nu h f 0 of the oxidizer minus 1 plus nu h f 0 of the products ok. The terms within the brackets you will immediately recognize is nothing, but the negative of the enthalpy change of this reaction which is nothing, but the negative of the enthalpy of combustion or the calorific value of the fuel.

So, this is simply the rate of consumption of the fuel times the enthalpy of combustion ok. The terms within the bracket is the negative of the enthalpy of the combustion. So, this will become negative delta H C and negative delta H C multiplied by negative omega dot F is delta H C.

Now, I hope it makes intuitive sense that the heat release because of combustion reactions return as sum negative sum of omega dot i h f i, for the simple case reduces to simply the rate of consumption of the fuel multiplied by the calorific value of the fuel which makes intuitive sense right. Is that clear, any questions? Yeah, all right. Let us go back to the conservation equations.